What is a "Point Group"?

Point Group Definition

- A classification scheme for finite objects (molecules)
- Molecules having the same set of symmetry elements/operations "belong to" the same point group
- Point groups have labels we will learn
- We will use the Schoenflies notation (spectroscopy) rather than the Hermann-Mauguin notation (crystallography)

Point Group Definition

- A classification scheme for finite objects (molecules)
- Molecules having the same set of symmetry elements/operations "belong to" the same point group
- Point groups have labels we will learn
- We will use the Schoenflies notation (spectroscopy) rather than the Hermann-Mauguin notation (crystallography)

Point Group Definition

- A classification scheme for finite objects (molecules)
- Molecules having the same set of symmetry elements/operations "belong to" the same point group
- Point groups have labels we will learn
- We will use the Schoenflies notation (spectroscopy) rather than the Hermann-Mauguin notation (crystallography)

Point Group Definition

- A classification scheme for finite objects (molecules)
- Molecules having the same set of symmetry elements/operations "belong to" the same point group
- Point groups have labels we will learn
- We will use the Schoenflies notation (spectroscopy) rather than the Hermann-Mauguin notation (crystallography)

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

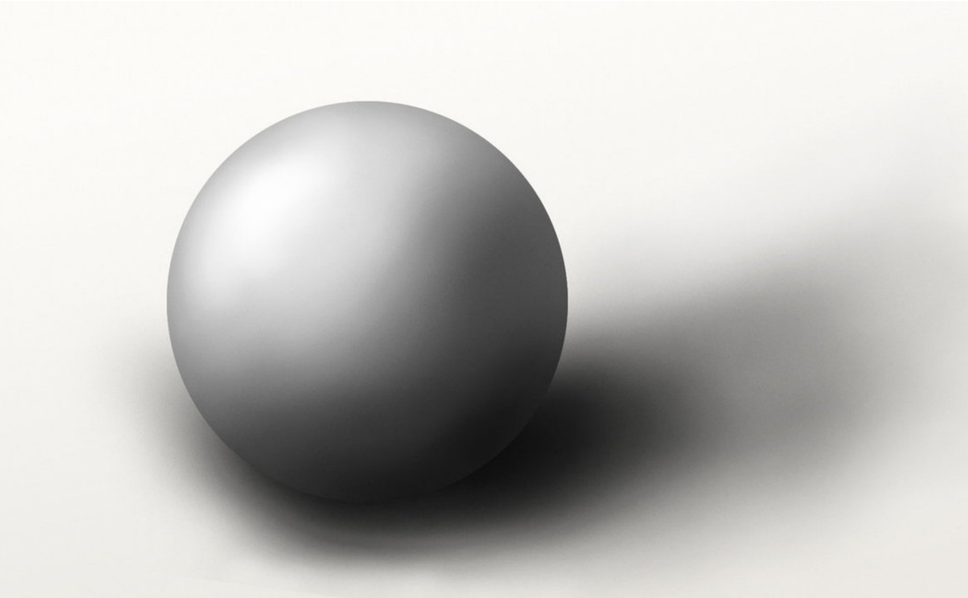
Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

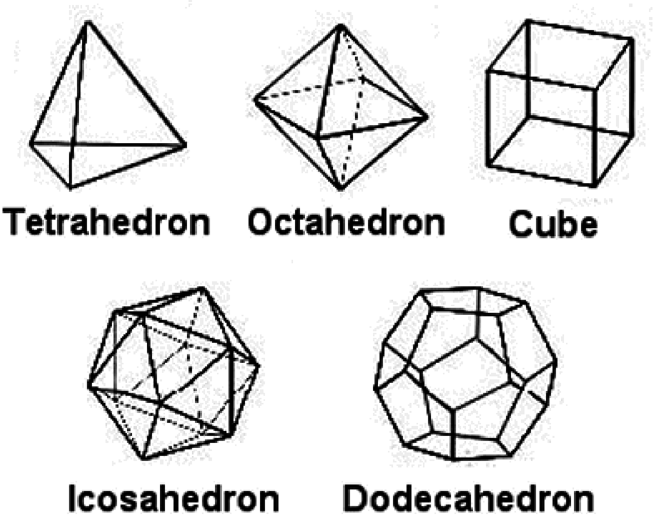
Types of Point Groups
Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n



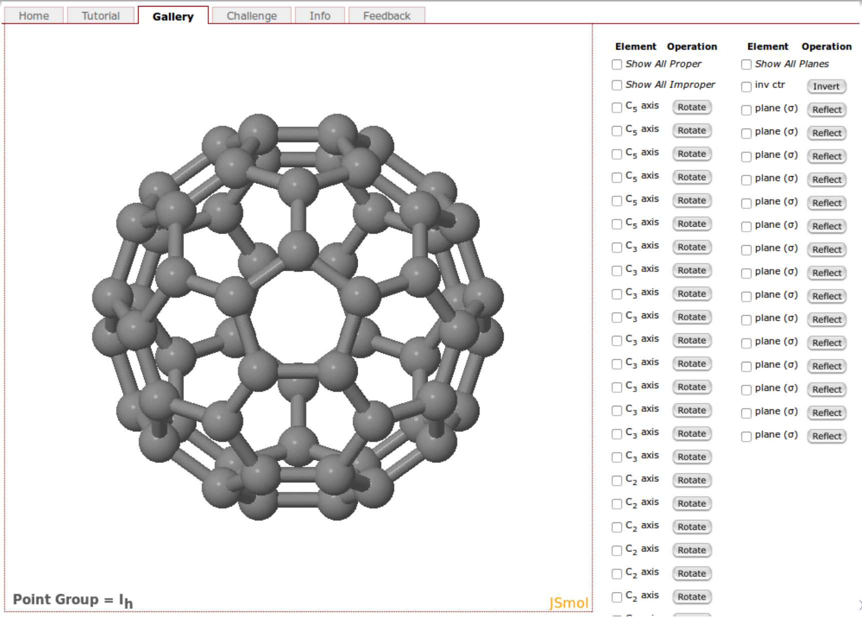
The Platonic Solids: Polyhedra with Regular Polygon Faces

Symmetry lowered from the sphere, but still present are multiple higher-order axes



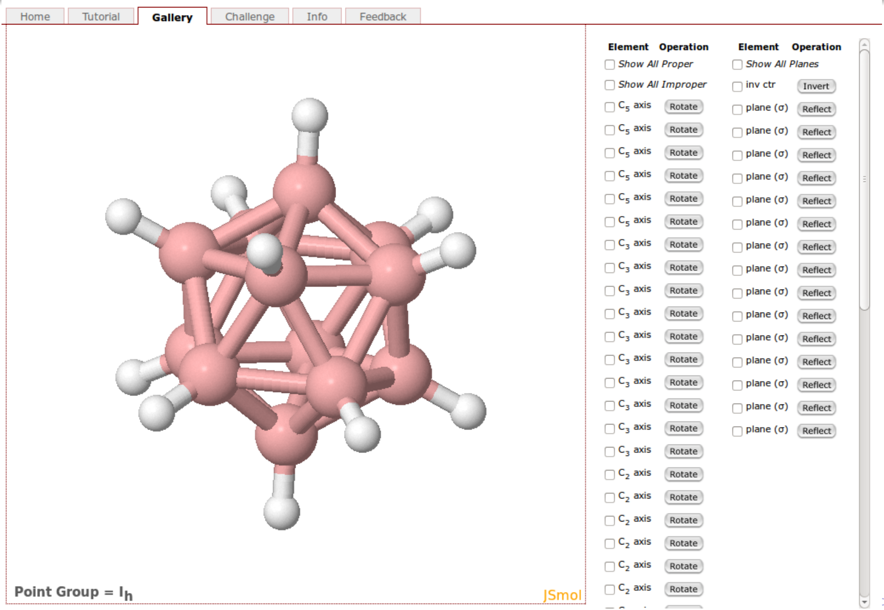
High Symmetry Groups

These have multiple higher order ($n > 2$) rotation axes. Example: C_{60}, icosahedral



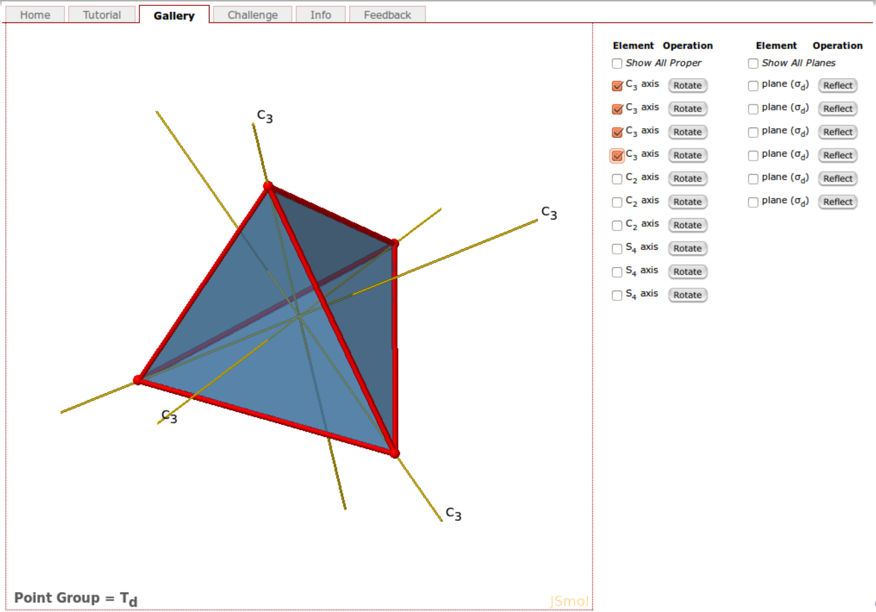
High Symmetry Groups

These have multiple higher order ($n > 2$) rotation axes. Example: $[B_{12}H_{12}]^{2-}$, icosahedral



High Symmetry Groups

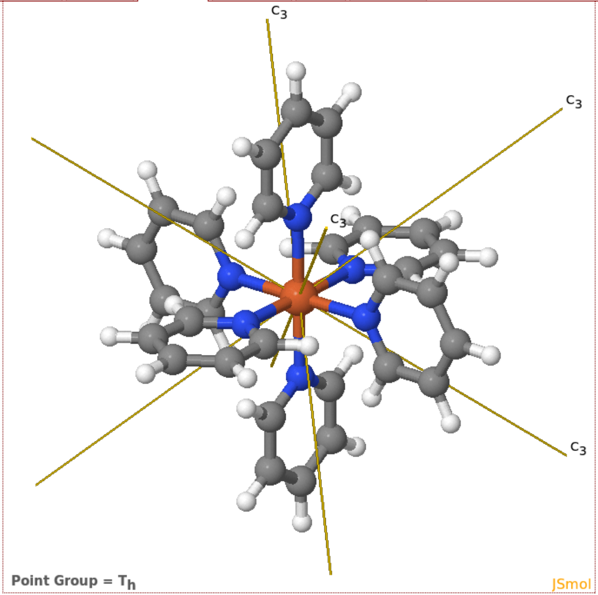
The tetrahedron has four C_3 axes but lacks inversion center



High Symmetry Groups

The group T_h has four C_3 axes (through octahedral faces) and adds the inversion center

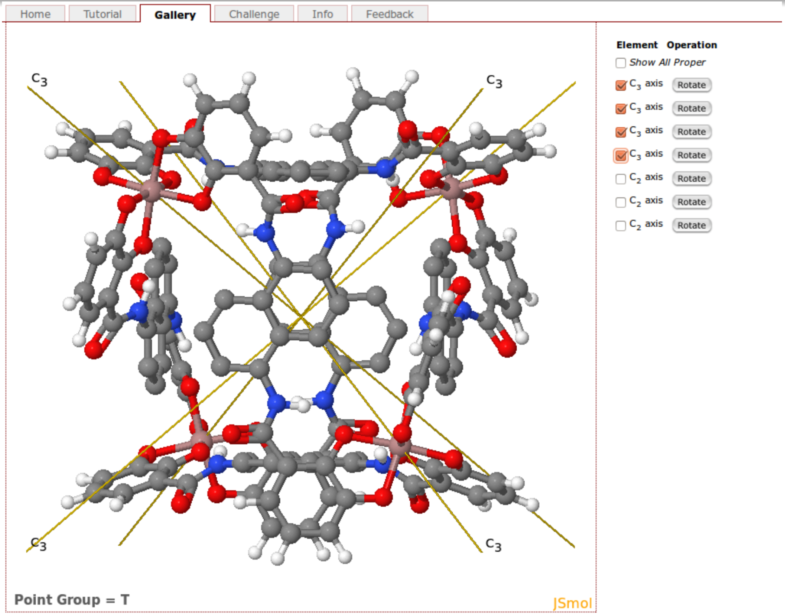
Home | Tutorial | **Gallery** | Challenge | Info | Feedback



Element	Operation	Element	Operation
Show All Proper		inv ctr	Invert
Show All Improper		plane (σ_h)	Reflect
C_3 axis	Rotate	plane (σ_h)	Reflect
C_3 axis	Rotate	plane (σ_h)	Reflect
C_3 axis	Rotate		
C_3 axis	Rotate		
C_2 axis	Rotate		
C_2 axis	Rotate		
C_2 axis	Rotate		
S_6 axis	Rotate		
S_6 axis	Rotate		
S_6 axis	Rotate		
S_6 axis	Rotate		

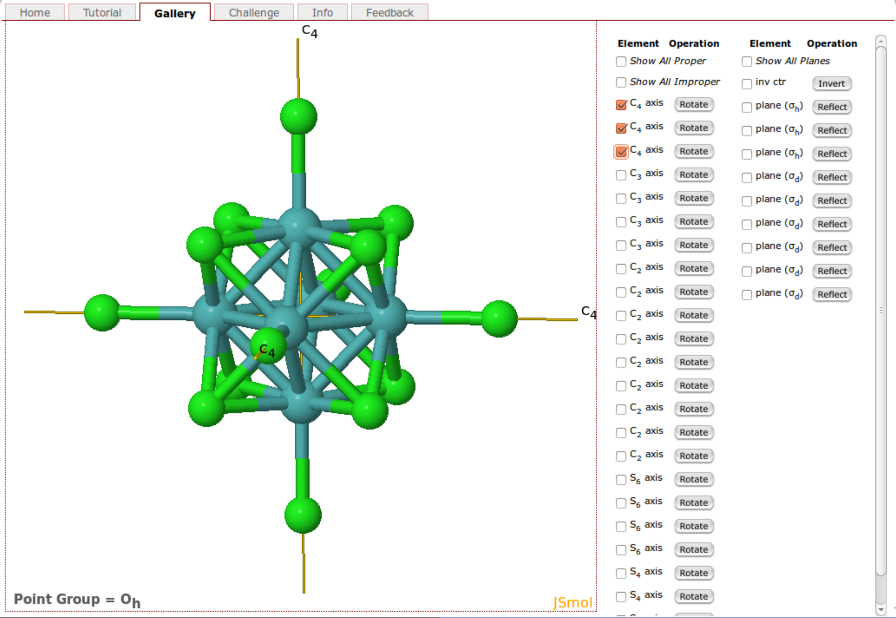
High Symmetry Groups

The group T is a pure rotation group with no mirror planes or inversion centers



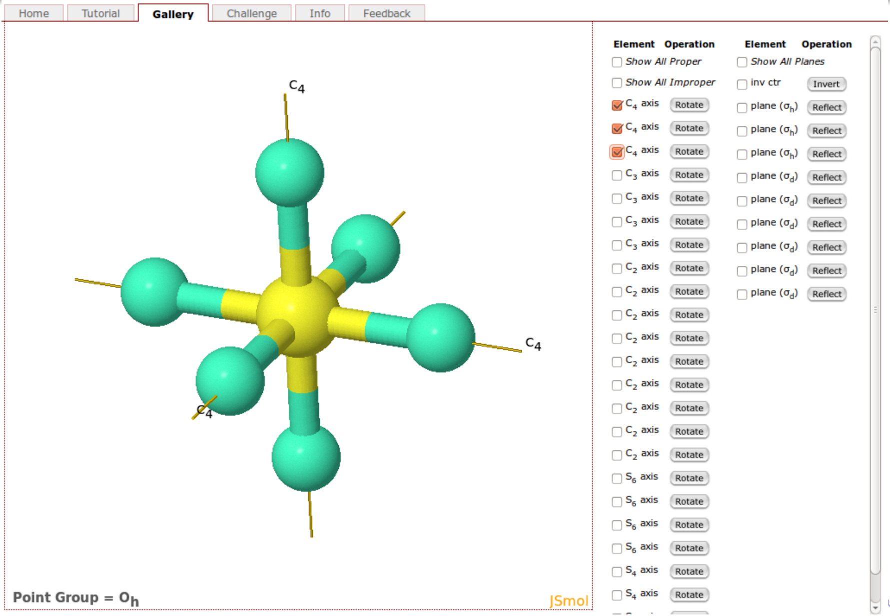
High Symmetry Groups

The group O_h has three C_4 axes and an inversion center: $[Mo_6Cl_{14}]^{2-}$



High Symmetry Groups

The group O_h has three C_4 axes and an inversion center: SF_6



Groups of Low Symmetry

The identity alone, or together with one mirror or an inversion center

- The identity only, C_1
- The identity plus one mirror plane: C_s
- The identity plus an inversion center: C_i

Groups of Low Symmetry

The identity alone, or together with one mirror or an inversion center

- The identity only, C_1
- The identity plus one mirror plane: C_s
- The identity plus an inversion center: C_i

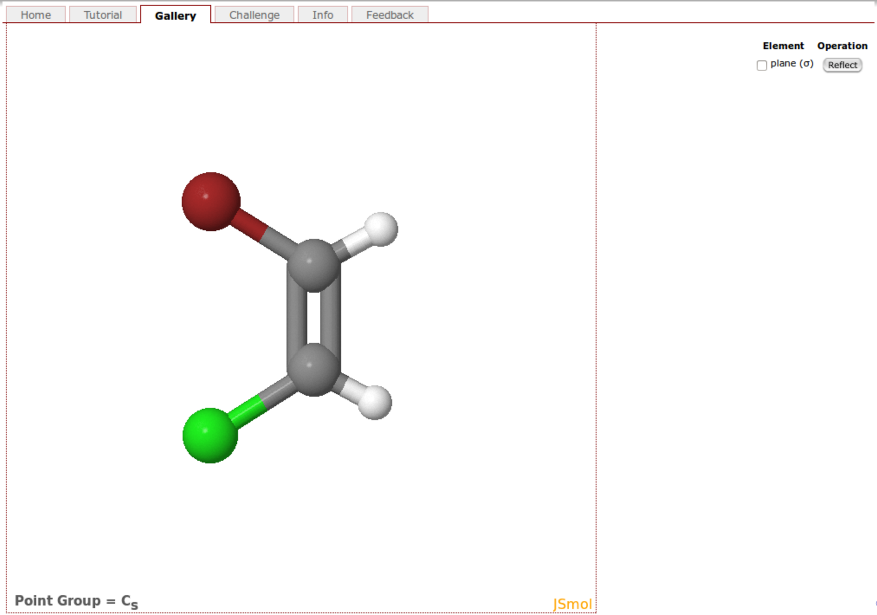
Groups of Low Symmetry

The identity alone, or together with one mirror or an inversion center

- The identity only, C_1
- The identity plus one mirror plane: C_s
- The identity plus an inversion center: C_i

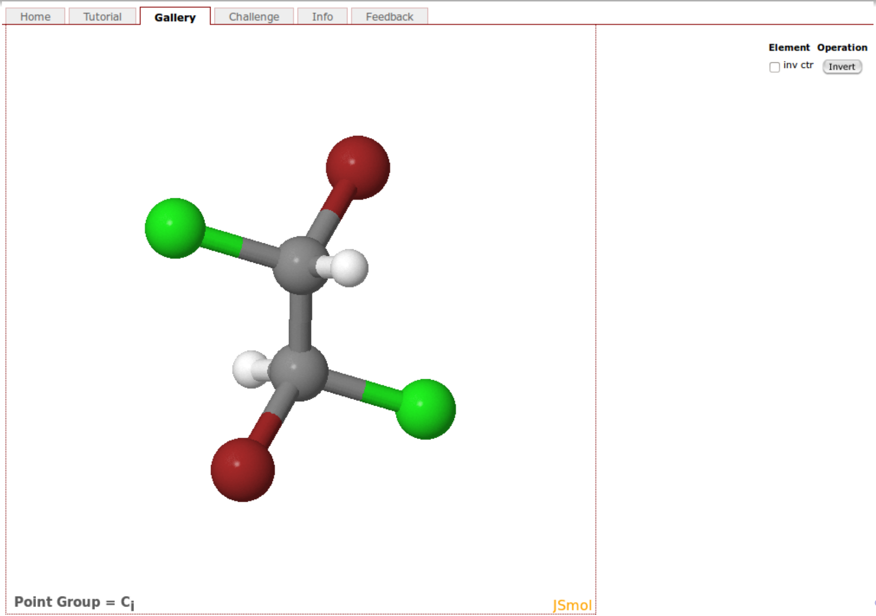
Groups of Low Symmetry

The identity alone, or together with one mirror or an inversion center



Groups of Low Symmetry

The identity alone, or together with one mirror or an inversion center



Linear Molecules

Distinguish based upon presence or absence of $\perp$ C_2 axes

- A linear molecule has a C_∞ axis of rotation
- Nitrous oxide, N_2O, N=N=O, the two ends are different so no C_2 $\perp$ to the C_∞, the point group assignment is $C_{\infty v}$
- Carbon dioxide, CO_2, O=C=O, the two ends are "symmetry related" and exchangeable by $\perp$ C_2 or by σ_h so the point group assignment is $D_{\infty h}$
- In general, D groups have nC_2 axes $\perp$ to the C_n (single principal rotation axis)

Linear Molecules

Distinguish based upon presence or absence of $\perp$ C_2 axes

- A linear molecule has a C_∞ axis of rotation
- Nitrous oxide, N_2O, N=N=O, the two ends are different so no C_2 $\perp$ to the C_∞, the point group assignment is $C_{\infty v}$
- Carbon dioxide, CO_2, O=C=O, the two ends are "symmetry related" and exchangeable by $\perp$ C_2 or by σ_h so the point group assignment is $D_{\infty h}$
- In general, D groups have nC_2 axes $\perp$ to the C_n (single principal rotation axis)

- A linear molecule has a C_∞ axis of rotation
- Nitrous oxide, N_2O, N=N=O, the two ends are different so no C_2 $\perp$ to the C_∞, the point group assignment is $C_{\infty v}$
- Carbon dioxide, CO_2, O=C=O, the two ends are "symmetry related" and exchangeable by $\perp$ C_2 or by σ_h so the point group assignment is $D_{\infty h}$
- In general, D groups have nC_2 axes $\perp$ to the C_n (single principal rotation axis)

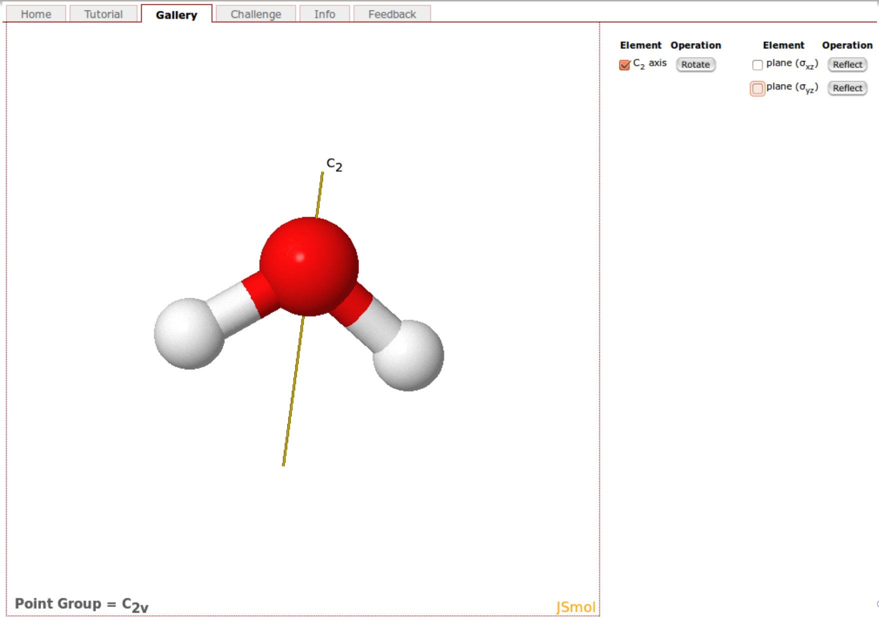
Linear Molecules

Distinguish based upon presence or absence of $\perp$ C_2 axes

- A linear molecule has a C_∞ axis of rotation
- Nitrous oxide, N_2O, N=N=O, the two ends are different so no $C_2 \perp$ to the C_∞, the point group assignment is $C_{\infty v}$
- Carbon dioxide, CO_2, O=C=O, the two ends are "symmetry related" and exchangeable by $\perp$ C_2 or by σ_h so the point group assignment is $D_{\infty h}$
- In general, D groups have nC_2 axes $\perp$ to the C_n (single principal rotation axis)

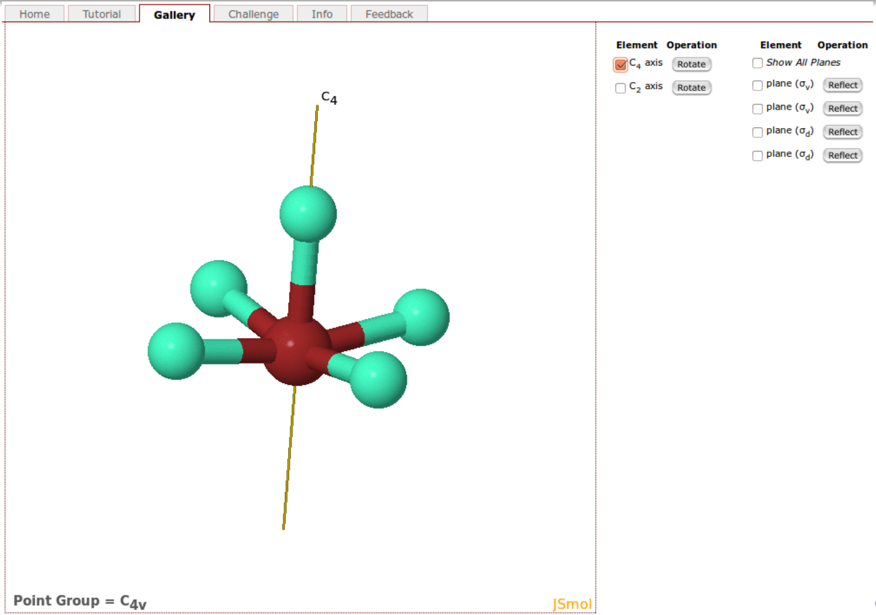
Examples of C groups

A single C_n plus n vertical mirror planes



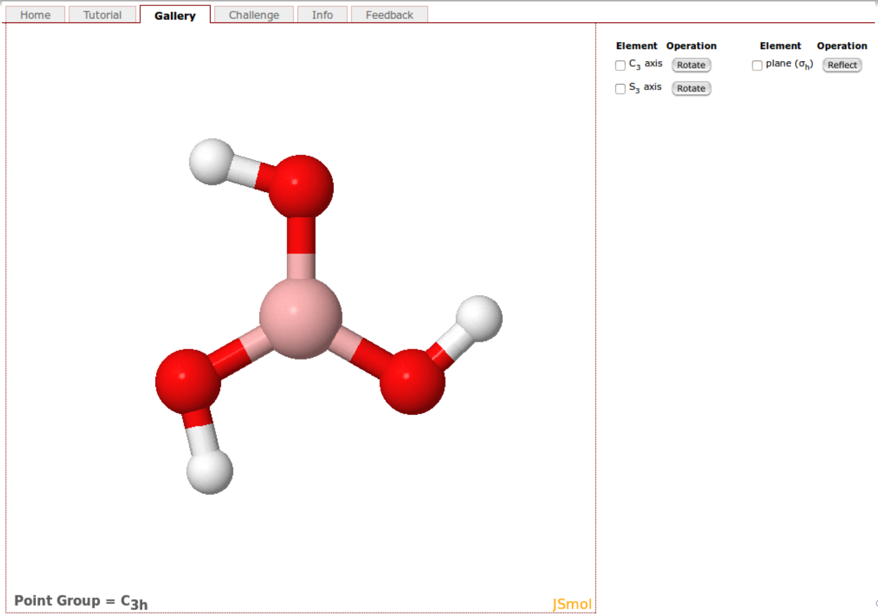
Examples of C groups

A single C_n plus n vertical mirror planes



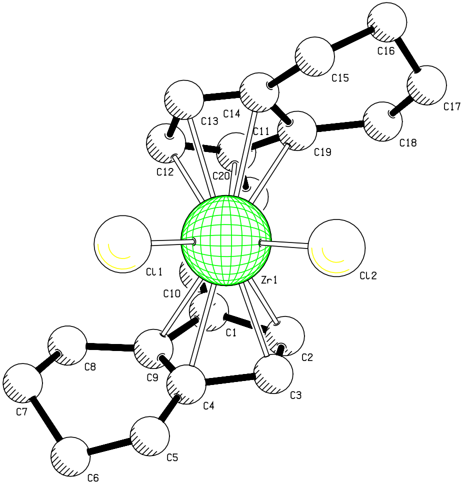
Examples of C groups

A single C_n plus a horizontal mirror plane



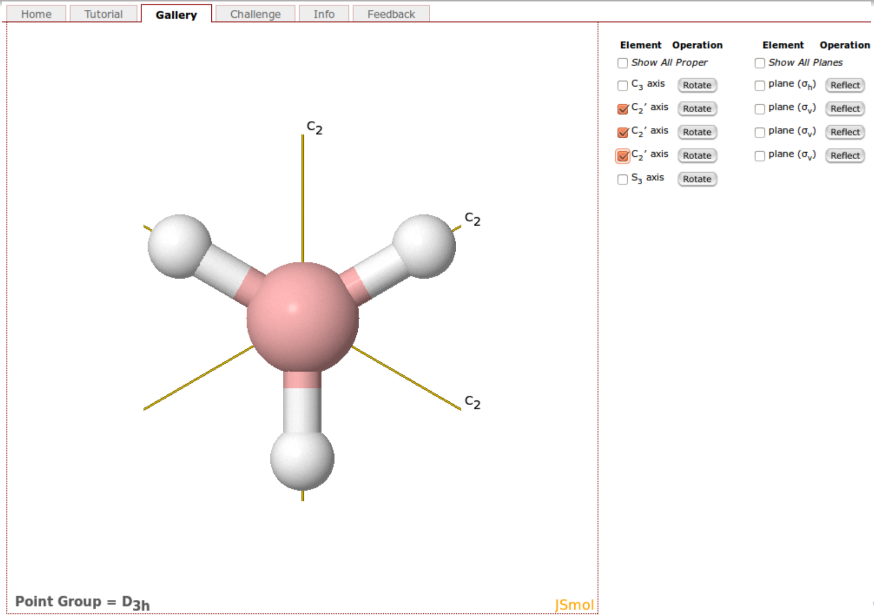
Examples of *C* groups

A single C_2 with no mirror planes: *ansa* metallocene example of point group C_2



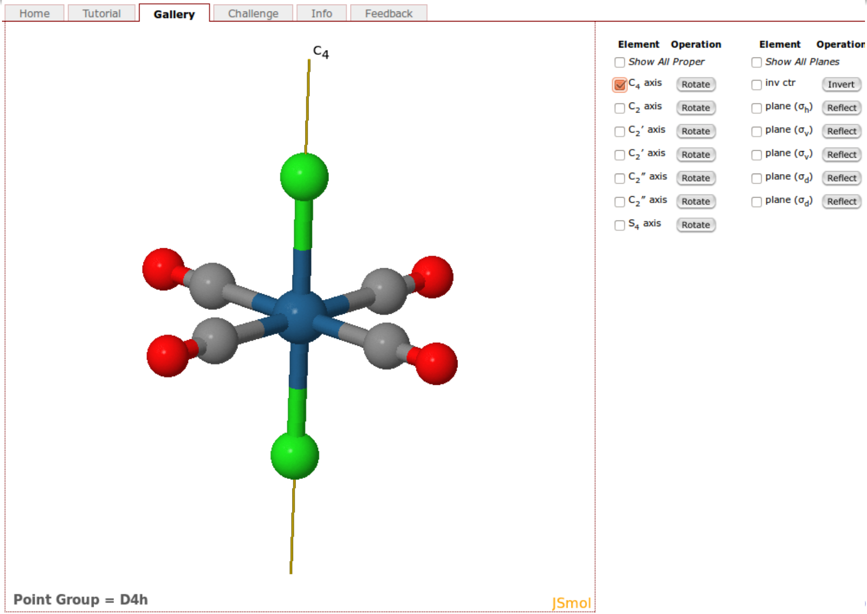
Examples of D groups

D_{nh} has n C_2 $\perp$ to the C_n, plus a σ_h



Examples of D groups

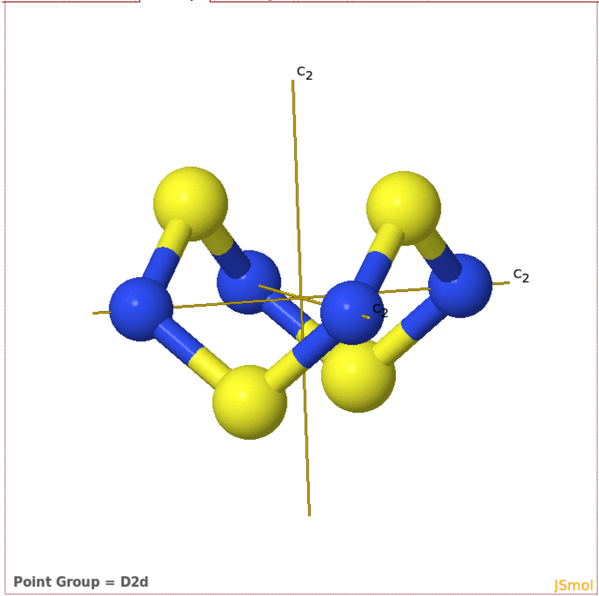
D_{nh} has n C_2 $\perp$ to the C_n, plus a σ_h



Examples of D groups

D_{nd} has n C_2 $\perp$ to the C_n, plus $n\sigma_d$ but no σ_h; example is S_4N_4

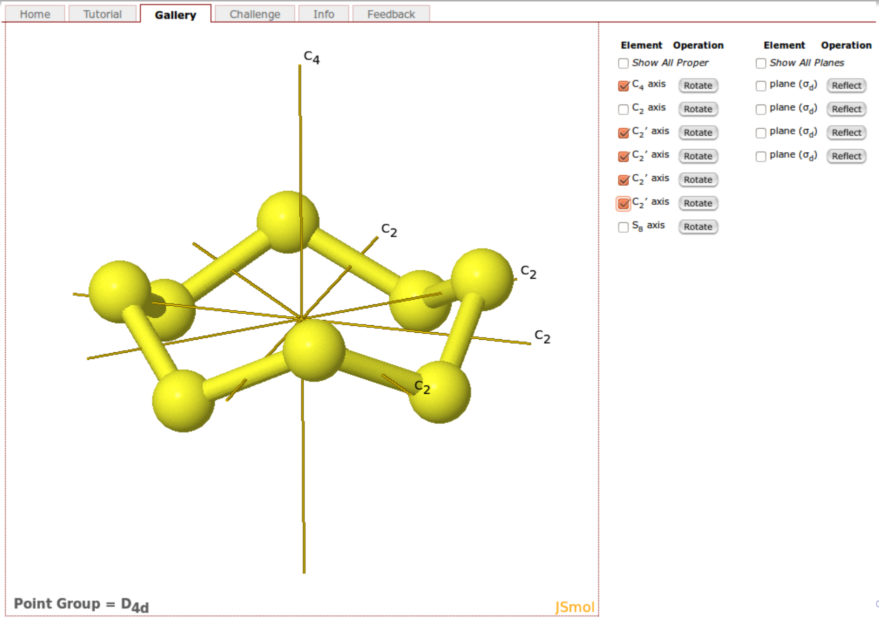
Home | Tutorial | **Gallery** | Challenge | Info | Feedback



Element	Operation	Element	Operation
C_2 axis	Rotate	plane (σ_d)	Reflect
C_2' axis	Rotate	plane (σ_d)	Reflect
C_2' axis	Rotate		
S_4 axis	Rotate		

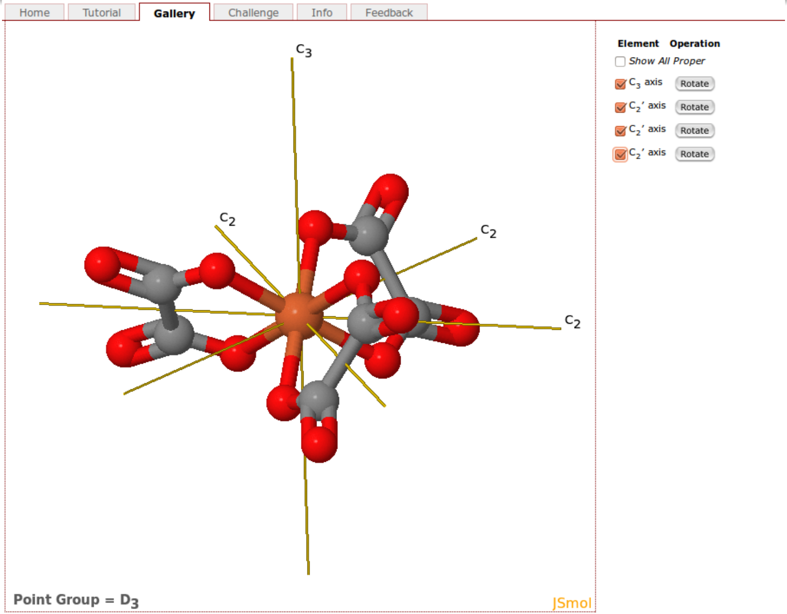
Examples of D groups

D_{nd} has n C_2 $\perp$ to the C_n, plus $n\sigma_d$ but no σ_h; example is S_8



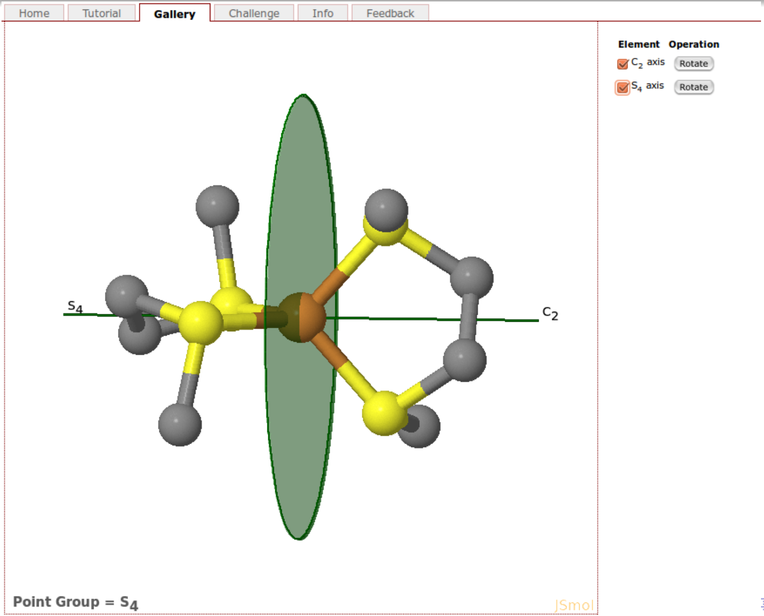
Examples of *D* groups

D_n has n C_2 $\perp$ to the C_n, but no mirror planes; example is $[Fe(C_2O_4)_3]^{3-}$



Example of S_n groups

S_n only for $n = 2, 4, 6, \ldots$ but note, S_2 = inversion so that is C_i



Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

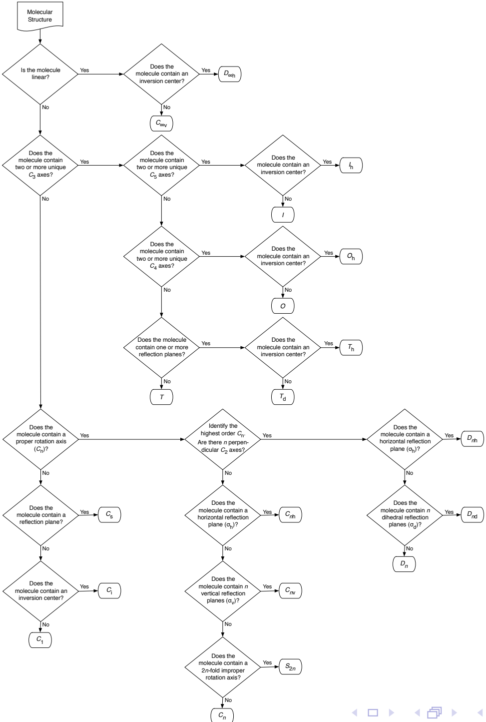
Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n

Types of Point Groups

Labels are the Schoenflies symbols: here are six limiting symmetry types

- High symmetry, multiple higher-order ($n > 2$) rotation axes. Examples: T_d, I_h, O_h
- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: C_1, C_s, C_i
- Linear molecules: $C_{\infty v}$, $D_{\infty h}$
- C groups: C_{nv}, C_{nh}, C_n
- D groups: D_{nd}, D_{nh}, D_n
- S groups: S_4, S_6, S_8, etc.; only operations present are based upon S_n



Molecular Structure
Is the molecule linear?
Yes
No
Does the molecule contain an inversion center?
Yes
$D_{\infty h}$
No
$C_{\infty v}$
Does the molecule contain two or more unique C_3 axes?
Does the molecule contain two or more unique C_5 axes?
Does the molecule contain an inversion center?
I_h
I
Does the molecule contain two or more unique C_4 axes?
Does the molecule contain an inversion center?
O_h
O
Does the molecule contain one or more reflection planes?
Does the molecule contain an inversion center?
T_h
T
T_d
Does the molecule contain a proper rotation axis (C_n)?
Identify the highest order C_n. Are there n perpendicular C_2 axes?
Does the molecule contain a horizontal reflection plane (σ_h)?
D_{nh}
Does the molecule contain n dihedral reflection planes (σ_d)?
D_{nd}
D_n
Does the molecule contain a reflection plane?
C_s
Does the molecule contain an inversion center?
C_i
C_1
Does the molecule contain a horizontal reflection plane (σ_h)?
C_{nh}
Does the molecule contain n vertical reflection planes (σ_v)?
C_{nv}
Does the molecule contain a 2n-fold improper rotation axis?
S_{2n}
C_n